

=> file reg

FILE 'REGISTRY' ENTERED AT 15:56:18 ON 09 FEB 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 8 FEB 2005 HIGHEST RN 827572-71-4

DICTIONARY FILE UPDATES: 8 FEB 2005 HIGHEST RN 827572-71-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

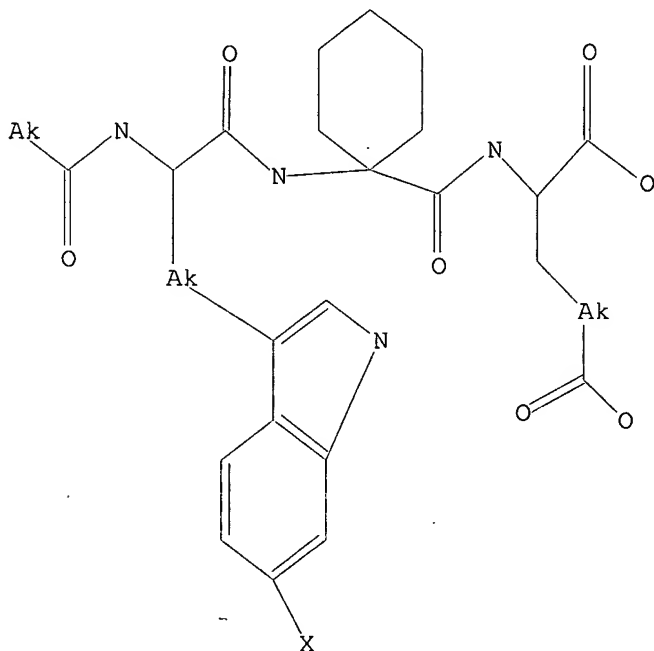
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d stat que l12

L10 STR



Note: In the full file search there were no structures that matched this.

Structure attributes must be viewed using STN Express query preparation.

L12 0 SEA FILE=REGISTRY SSS FUL L10

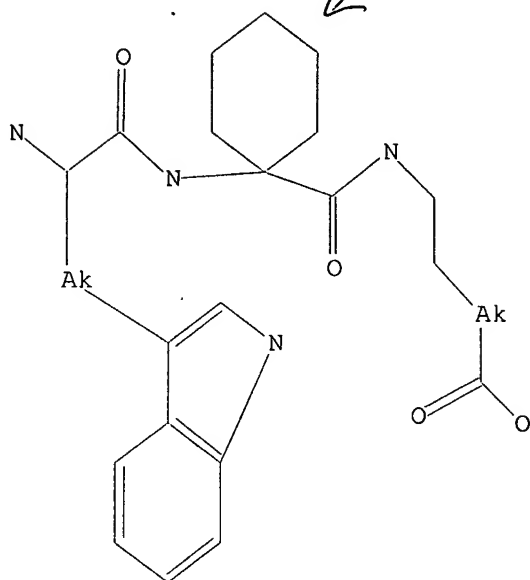
100.0% PROCESSED 1818 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

=> d stat que 117
L15 STR

This appears to be the unique element.



Note: I broadened the search, eliminating some structural elements from the first search - there were still no matches in the full file search.

Structure attributes must be viewed using STN Express query preparation.
L17 0 SEA FILE=REGISTRY SSS FUL L15

100.0% PROCESSED 5877 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

=> d que 119
L18

nr = number of rings

213 SEA FILE=REGISTRY ABB=ON PLU=ON C=25 AND N=4 AND O=7 AND
NR=3 AND NRS=2

L19

12 SEA FILE=REGISTRY ABB=ON PLU=ON L18 AND CL=1

I scanned these 12 structures - no matches

=> d que 120

L18

213 SEA FILE=REGISTRY ABB=ON PLU=ON C=25 AND N=4 AND O=7 AND
NR=3 AND NRS=2

L20

3 SEA FILE=REGISTRY ABB=ON PLU=ON L18 AND BR=1

No matches here either - the 3d ring in both cases is normalized not single bonded.

=> file home

FILE 'HOME' ENTERED AT 15:57:49 ON 09 FEB 2005

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